(FILE 'HOME' ENTERED AT 14:25:47 ON 28 MAR 2007)

FILE 'REGISTRY' ENTERED AT 14:25:54 ON 28 MAR 2007

L1 STRUCTURE UPLOADED

L2 12 S L1 SSS SAM

L3 . 197 S L1 SSS FUL

FILE 'CAPLUS, USPATFULL, PCTFULL' ENTERED AT 14:27:41 ON 28 MAR 2007

FILE 'CAPLUS, USPATFULL' ENTERED AT 14:27:55 ON 28 MAR 2007

L4 20 S L3

=> log hold

C:\Program Files\Stnexp\Queries\vancomycin core #3.str

chain nodes :

12-41 21-25 30-40 35-79

normalized bonds :

55-56

```
17
                        27
                                41
                                    42
                                       63
                                               65
                                                      77
      16
                            40
             18
                 25
                     26
                                           64
                                                   76
                                                          78
                                                              79
                                                                  80
                                                                     81
                                                                         82
                                                                             83
ring nodes :
                          10
                             11
                                 12
                                     13
                                        14
                                            15
                                                19
                                                    20
                                                       21
                                                           22
                                                               23
                                                                   24
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       33
                  36
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       58
                      62
               60
                  61
                          66
                             67
                                 68
                                     69
                                         70
                                            71
                                                72
                                                    73
                                                           75
chain bonds :
   4-9 9-10 12-41 13-17 14-18 15-16 16-19 21-25 22-26 23-27 30-40 35-79 41-42
   43-83 45-82 50-64 52-63 54-65 61-81 67-80 70-78 73-77 75-76
ring bonds :
   1-2 1-6 1-68 2-3 3-4 3-8 4-5 5-6 5-7 7-29 8-28 10-11 10-15 11-12 12-13
   13-14 14-15 19-20 19-24 20-21 21-22 22-23 23-24 28-30 28-34 29-35 29-39
   30-31 31-32 32-33 32-43 33-34 35-36 36-37 37-38 37-75 38-39 43-44 44-45
                      47-48 48-49 48-53 49-50 49-55 50-51 51-52 52-53 54-55
   44-62 45-46 46-47
   54-59 55-56 56-57
                      57-58 57-60 58-59 60-61 60-66 61-62 66-67 67-68 68-69
   69-70 70-71 71-72
                      72-73 73-74 74-75
exact/norm bonds :
   1-68 3-8 4-9 5-7 7-29 8-28 9-10 10-11 10-15 11-12 12-13 13-14 13-17 14-15
   14-18 15-16 16-19
                      19-20 19-24 20-21 21-22 22-23 22-26 23-24 23-27 32-43
                      43-83 44-45 44-62 45-46 45-82 46-47 47-48 49-55 50-64
   37-75 41-42 43-44
   52-63 54-65 57-60 60-61 60-66 61-62 61-81 66-67 67-68 67-80 68-69 69-70
   70-71 70-78 71-72 72-73 73-74 73-77 74-75 75-76
exact bonds :
```

1-2 1-6 2-3 3-4 4-5 5-6 28-30 28-34 29-35 29-39 30-31 31-32 32-33 33-34

35-36 36-37 37-38 38-39 48-49 48-53 49-50 50-51 51-52 52-53 54-55 54-59

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 17:CLASS 18:CLASS 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:CLASS 26:CLASS 27:CLASS 28:Atom 29:Atom 30:Atom 31:Atom 32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:CLASS 41:CLASS 42:Atom 43:Atom 44:Atom 45:Atom 46:Atom 47:Atom 48:Atom 49:Atom 50:Atom 51:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:Atom 57:Atom 58:Atom 59:Atom 60:Atom 61:Atom 62:Atom 63:CLASS 64:CLASS 65:CLASS 66:Atom 67:Atom 68:Atom 69:Atom 70:Atom 71:Atom 72:Atom 73:Atom 74:Atom 75:Atom 76:CLASS 77:CLASS 78:CLASS 79:CLASS 80:CLASS 81:CLASS 82:CLASS 83:CLASS